

Visual Grid Programming For Application Scientists

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Problem

- Current interfaces to Grid and Collaborative technologies are too complex for most application scientists.
 - Very steep learning curve.
 - Often times perceived as easier to develop a one-off solution then to adopt standard middleware tools.
 - Provides a major barrier to wide-spread adoption.
- Poor integration between collaborative tools and Grid middleware.

High-Level Goals

- Provide tools that the scientific community is already familiar with.
- Provide high-level interfaces that capture common scientific tasks.
- Integrate collaborative tools directly.
- Recognize that application scientists have a wide variety of CS knowledge.
 - Expert users who can program their own tools.
 - Sophisticated users that can extend existing tools.
 - Normal users of tools.
- No single solution will be appropriate for all situations!

High-Level Abstractions

- What have we tried?
 - High-Level programming languages and abstractions
 - Useful for expert users, but too complex for many.
 - Domain specific abstractions increase the usability for moderately sophisticated users.
 - An important component for developing Visual Programming environments.
 - Portals
 - Very useful for providing easy to use interfaces for many users.
 - Excellent for collaboration.
 - Can be very difficult to customize for the sophisticated users.
 - It is very challenging to do highly interactive interfaces.

Visual Programming (VP)

- For many scientific applications it is natural to model their process visually.
 - Can easily drag and drop components to construct a variety of different experiments.
 - Networks can be shared amongst collaborators.
 - Need to support both modeling data and control flows.
- Many scientists are already familiar with this model from tools like AVS®.



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Example VP Environment



The screenshot displays a computer interface for molecular simulation. The main window is UCSF Chimera, showing a 3D model of a protein-ligand complex. Below the model is a command line and a list of active models. To the right is the NODE EDITOR window, which contains a palette of simulation steps: File, Load PDB, psfgen, minimize, solvate and neutralize, Enter # steps, equilibrate solvent, production dynamics, postprocess trajectory, and realtime monitoring. Below the Node Editor is the NETWORK EDITOR window, which shows a workflow diagram. The workflow starts with 'Enter file name' (1f88.pdb) leading to 'Load PDB', then 'psfgen', 'minimize', 'solvate and neutralize', 'production dynamics', and 'realtime monitoring'. The 'Enter # steps' is set to 1000. The bottom of the screen shows a taskbar with various icons and a system tray with the time 22:20.

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VP Requirements

- Implement in a high-level, interpreted, simple to use language that has support in the scientific community.
- Must integrate with the next generation of Grid Services, e.g., WS-RF.
 - WS-RF makes introspection for service composition significantly easier.
 - This allows for late binding which is vitally important in a dynamic Grid environment.

VP Requirements

- Support the integration of collaborative technologies to allow for shared visual development.
 - Could be integrated in a portal, or used with the Access Grid, etc.
- Use high-level abstractions to allow submission to multiple execution engines.
 - Direct Globus submissions.
 - DAGMan from the Condor Project.
 - BPEL4WS, or other emerging standards.

Why Interpreted Languages

- Easier to support the three classes of users mentioned earlier.
 - Expert application scientists will customize the general framework for their domain.
 - Interpreted languages significantly lower the barrier to doing this by shortening development and debug time.
 - Sophisticated users will be able to customize the domain specific tool.
 - Interpreted languages support the ability to dynamically edit visual nodes on the fly using simplified interfaces.
- Well suited to integrating existing components.
 - Faster and easier to develop with.



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Dynamic Customization



nedelson's X desktop (bosshog.lbl.gov:1)

NETWORK EDITOR

File Edit Job Control

RUN STOP CONNECT DISCONNECT

Enter file name
1f88.pdb

Load PDB

psfgen

minimize

solvate and neutralize

production dynamics

realtime monitoring

Enter # steps
2000

Enter # steps
1000

Click on Run when network is completed

NODE EDITOR

File

label button 0 node

File name Load PDB psfgen

minimize solvate and neutralize Enter # steps

equilibrate solvent production dynamics postprocess trajectory

realtime monitoring

Editing minimize node

```
2
3 def __init__(self):
4     import gov.lbl.dsd.netlogger as netlogger
5     nl_flags = netlogger.OutputFlags.ULM | netlogger.OutputFlags.FLUSH
6     nldest = "x-netlog://bosshog.lbl.gov14845"
7     self.nl = netlogger.open(nldest,
8                             program='mini',
9                             flags=nl_flags,
10                            backup='/tmp/minibackup.log')
11
12     from NAMDTTools import NAMDMINimizer
13     NAMDMINimizer.dcdFreq = 500
14     NAMDMINimizer.outputTiming = 1000
15     NAMDMINimizer.cutoff = 8.0
16
17 def run(self, args):
18     self.nl.write(1, "sample.start", "val=%s", str(time.time()))
19     self.minimizer.run( inputs.get("NUMSTEPS"))
20     self.nl.write(1, "sample.end", "val=%s", str(time.time()))
21
```

Virtual

NETWOR

NOE

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Conclusions

- Research is necessary to develop better ways to allow scientists to interact with distributed Grid Services.
- No one solution will fit all users.
- Grid programming environments must support the collaborative nature of science today.

Conclusions

- A properly designed Visual Programming environment can meet the needs of many application scientists.
 - Requires the CS community to develop generic frameworks that can easily be customized by expert application scientists for their specific domain.
 - Must also support the ability of non-expert programmers to modify the domain specific environment to fit their specific needs.